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(FILE 'HOME' ENTERED AT 12:48:49 ON 16 FEB 2000)

FILE 'CA' ENTERED AT 12:49:00 ON 16 FEB 2000

L1 7853 S ISOTOP?(3A) (LABEL? OR TAG? OR MARK?)  
L2 702 S L1 AND (SPECIE OR SPECIAT?)  
L3 1182 S L1 AND (CHROM? OR SELEN? OR CR50 OR 50CR OR CR53 OR 53CR)  
L4 97 S L2 AND L3  
L5 223 S L2 AND (ISOTOP?(1A) DILUT? OR MIXTURE OR REDOX OR AUTOOX? OR FOLLOW?  
OR (DUAL OR DOUBLE) / TI)  
L6 255 S L4-5 NOT PY>1997  
L7 215 S L6 NOT RADIO?  
L8 40 S L6 NOT L7  
L9 3 S L8 AND (REPLAC? OR (SOIL AND SELEN?))  
L10 218 S L7, L9

=> d 110 bib, ab 1-218

L10 ANSWER 19 OF 218 CA COPYRIGHT 2000 ACS  
AN 126:168747 CA  
TI Trace quantification of the oxidative damage products, meta- and ortho-tyrosine, in biological samples by gas chromatography-electron capture negative ionization mass spectrometry  
AU Blount, Benjamin C.; Duncan, Mark W.  
CS Biomedical Mass Spectrometry Unit, Univ. New South Wales, Sydney, Australia  
SO Anal. Biochem. (1997), 244(2), 270-276 CODEN: ANBCA2; ISSN: 0003-2697  
DT Journal  
LA English  
AB Oxygen radicals damage biomols. and may contribute to cellular aging and degenerative disease. We describe a sensitive method for the quantification of two endogenous biomarkers of oxidative damage: meta-tyrosine (m-Tyr) and ortho-tyrosine (o-Tyr). The assay can be applied to direct anal. of free amino acids or protein-bound amino acids following hydrolysis. The assay involves derivatization with pentafluorobenzyl bromide and extn. into n-decane, followed by gas chromatog.-mass spectrometry. Stable isotope labeled m- and o-Tyr (2H4) and phenylalanine [i.e., Phe (2H5)] were added as internal stds. to improve anal. accuracy. Quantification of as little as 50 pg of m- and o-Tyr in 100 µg protein is possible and the data are expressed as a molar ratio of m- and o-Tyr to native Phe. The assay was used to det. the levels of m- and o-Tyr in freshly isolated human plasma protein (4.05±0.67 m-Tyr per 104 Phe, 0.35±0.07 o-Tyr per 104 Phe). Exposure of human plasma to reactive oxygen species significantly increased the levels of m-Tyr (56.4±1.1 m-Tyr per 104 Phe) and o-Tyr (48.9±1.3 o-Tyr per 104 Phe). The mild hydrolysis and derivatization conditions caused no artifactual formation of either m- or o-Tyr.

L10 ANSWER 24 OF 218 CA COPYRIGHT 2000 ACS  
AN 125:113117 CA  
TI Chemical methods for assessing systemic exposure to dietary heterocyclic amines in man  
AU Davies, Donald S.; Gooderham, Nigel J.; Murray, Stephen; Lynch, Anthony; De La Torre, Rafael; Segura, Jorge; Boobis, Alan R.  
CS Department Clinical Pharmacology, Royal Postgraduate Medical School, London, W12 0NN, UK  
SO Arch. Toxicol., Suppl. (1996), 18 (Toxicology--From Cells to Man), 251-258  
CODEN: ATSUDG; ISSN: 0171-9750  
DT Journal *moder*

LA English  
AB A significant proportion of the mutagenic material present in cooked beef is accounted for by 2-amino-3,8-dimethylimidazo[4,5-f]quinoxaline (MeIQx) and 2-amino-1-methyl-6-phenylimidazo[4,5-b]pyridine (PhIP) which are formed during cooking of meat. N-hydroxylation catalyzed by CYP1A2 is the major pathway of metab. of MeIQx and PhIP and is solely responsible for the generation of mutagenic species. Assays for MeIQx and PhIP in foods and body fluids were developed utilizing gas chromatog./mass spectrometry with stable isotope labeled analogs as internal stds. Studies using these assays have demonstrated that both MeIQx and PhIP are well absorbed and extensively metabolized following ingestion of amine-contg. beef by humans. Studies in which furafylline, a potent and selective inhibitor of human CYP1A2, was administered before ingestion of beef revealed that more than 90% of MeIQx and 70% of PhIP are N-hydroxylated in vivo, probably pre-systemically in the liver. The results demonstrate that unchanged MeIQx and PhIP in urine are accurate and sensitive measures of systemic exposure to the amines.

L10 ANSWER 50 OF 218 CA COPYRIGHT 2000 ACS  
AN 120:199041 CA  
TI Airborne measurements of sulfur dioxide, dimethyl sulfide, carbon disulfide, and carbonyl sulfide by isotope dilution gas chromatography/mass spectrometry  
AU Bandy, Alan R.; Thornton, Donald C.; Driedger, Arthur R., III  
CS Chem. Dep., Drexel Univ., Philadelphia, PA, USA  
SO J. Geophys. Res., [Atmos.] (1993), 98(D12), 23423-33 CODEN: JGRDE3; ISSN: 0148-0227  
DT Journal *order*  
LA English  
AB A gas chromatograph/mass spectrometer is described for detg. atm. sulfur dioxide, carbon disulfide, di-Me sulfide, and carbonyl sulfide from aircraft and ship platforms. Isotopically labeled variants of each analyte were used as internal stds. to achieve high precision. The lower limit of detection for each species for an integration time of 3 min was 1 pptv for sulfur dioxide and di-Me sulfide and 0.2 pptv for carbon disulfide and carbonyl sulfide. All four species were simultaneously detd. with a sample frequency of one sample per 6 mi or greater. When only one or two species were detd., a frequency of one sample per 4 min was achieved. Because a calibration is included in each sample, no sep. calibration sequence was needed. Instrument warmup was only a few minutes. The instrument was robust in field deployments, requiring little maintenance.

L10 ANSWER 63 OF 218 CA COPYRIGHT 2000 ACS  
AN 118:195439 CA  
TI Key sulfur-containing compounds in the atmosphere and ocean. Determination by gas chromatography-mass spectrometry and isotopically labeled internal standards  
AU Bandy, Alan R.; Thornton, Donald C.; Ridgeway, Robert G., Jr.; Blomquist, Byron W.  
CS Chem. Dep., Drexel Univ., Philadelphia, PA, 19104, USA  
SO ACS Symp. Ser. (1992), 502(Isot. Eff. Gas-Phase Chem.), 409-22 CODEN: ACSMC8; ISSN: 0097-6156  
DT Journal *order*  
LA English  
AB Gas chromatog./mass spectrometric (GC/MS) methods using isotopically labeled internal stds. (GC/MS/ILS) are described for detg. atm. SO<sub>2</sub>, DMS, CS<sub>2</sub>, DMSO, di-Me sulfone (DMSO<sub>2</sub>) and COS and aq. DMS and DMSO. GC/MS/ILS has great immunity to variations in sampling efficiency and changes in

detector sensitivity. Using cryogenic preconcn. and integration times of 3 min, lower limits of detection are <1 ppt for these gas phase species. Lower limits of detection for aq. phase measurements are <1 pmol. Measurement precision is limited by either the lower limit of detection or the repeatability of the addn. of the std. Accuracy is detd. primarily by the accuracy of the stds. GC/MS/ILS appears to have the sensitivity and precision to make real time isotopic ratio measurements.

L10 ANSWER 68 OF 218 CA COPYRIGHT 2000 ACS

AN 118:141300 CA

TI Quantitative determination of oxidative base damage in DNA by stable isotope-dilution mass spectrometry

AU Dizdaroglu, Miral

CS Chem. Sci. Technol. Lab., Natl. Inst. Stand. Technol., Gaithersburg, MD, 20899, USA

SO FEBS Lett. (1993), 315(1), 1-6 CODEN: FEBLAL; ISSN: 0014-5793

DT Journal

LA English

AB The present study describes the quantification of modified bases in DNA by isotope-diln. mass spectrometry with the use of stable isotope-labeled analogs as internal stds. A no. of isotopically labeled DNA bases were synthesized. The mass spectra of their trimethylsilyl derivs. were recorded. Calibration plots were obtained for known quantities of modified bases and their isotope-labeled analogs. Quantification of various modified DNA bases by isotope-diln. mass spectrometry was demonstrated in isolated chromatin exposed to ionizing radiation. The results indicate that gas chromatog./stable isotope-diln. mass spectrometry is an ideally suited technique for selective and sensitive quantification of modified bases in DNA.

L10 ANSWER 69 OF 218 CA COPYRIGHT 2000 ACS

AN 118:138967 CA

TI Mass transport and calibration in liquid chromatography particle beam mass spectrometry

AU Ho, James S.; Behymer, Thomas D.; Budde, William L.; Bellar, Thomas A.

CS Environ. Monitor. Syst. Lab., U.S. Environ. Protect. Agency, Cincinnati, OH, USA

SO J. Am. Soc. Mass Spectrom. (1992), 3(6), 662-71 CODEN: JAMSEF; ISSN: 1044-0305

DT Journal

LA English

AB Differences in the designs of two liq. chromatog. particle beam mass spectrometry systems result in differences in the transport of ammonium acetate and differences in ion abundance-enhancing carrier effects. The effect of mobile phase compn., esp. the proportion of water in the mobile phase, on transport efficiency is described. Instrument detection limits for 12 compds. with two different interface designs are presented. The calibrations are generally nonlinear explained in terms of mass transport effects and supported by expts. with isotopically labeled species that coelute with the native species. Summary results of a small multilab. study are presented. Calibration with isotopically labeled internal stds. is recommended for real-world environmental samples.

L10 ANSWER 70 OF 218 CA COPYRIGHT 2000 ACS

AN 118:130813 CA

TI Grab sampling for the determination of sulfur dioxide and dimethyl sulfide in air by isotope dilution gas chromatography/mass spectrometry

AU Blomquist, Byron W.; Bandy, Alan R.; Thornton, Donald C.; Chen, Shaoming

CS Dep. Chem., Drexel Univ., Philadelphia, PA, 19104, USA  
SO J. Atmos. Chem. (1993), 16(1), 23-30 CODEN: JATCE2; ISSN: 0167-7764  
DT Journal  
LA English *order*

AB Developments allowing the direct detn. of SO<sub>2</sub> and Me<sub>2</sub>S in grab samples by gas chromatog./mass spectrometry with isotopically labeled stds. (GC/MS/ILS) are reported. Isotopomers of Me<sub>2</sub>S and SO<sub>2</sub> are used as internal stds. Spiked air samples are dried to a dew point of <-60° and trapped cryogenically in loops of Teflon tubing. Sealed samples are transported to the lab. under liq. N and later subjected to GC/MS anal. Holding times of ≤1 mo do not result in significant sample loss. For samples collected in a clean marine environment, concns. of SO<sub>2</sub> and Me<sub>2</sub>S >5 and 8 pptv (parts per trillion by vol.), resp., are significantly different from blanks at the 95% confidence level. Av. measurement precision derived from a propagation of errors are 9% for SO<sub>2</sub> and 42% for Me<sub>2</sub>S at concns. 5-15 pptv. Improvements are outlined which should provide sensitivity and precision comparable to that of on-site GC/MS. The technique will allow increased flexibility for the detn. of trace S species in the field under conditions where deployment of a mass spectrometer is not possible.

L10 ANSWER 79 OF 218 CA COPYRIGHT 2000 ACS  
AN 116:251438 CA

TI Preliminary study of metals in proteins by high-performance liquid chromatography-inductively coupled plasma mass spectrometry using multi-element time-resolved analysis

AU Owen, Linda M. W.; Crews, Helen M.; Hutton, Robert C.; Walsh, Amanda  
CS Inst. Environ. Biol. Sci., Lancaster Univ., Lancaster, LA1 4YQ, UK  
SO Analyst (London) (1992), 117(3), 649-55 CODEN: ANALAO; ISSN: 0003-2654  
DT Journal  
LA English

AB The feasibility of multielement and multiisotope detns. during the online chromatog. sepn. of protein matrixes was investigated using time-resolved software with inductively coupled plasma mass spectrometry. Size-exclusion chromatog. was used to sep. a mixt. of known proteins and the behavior of assocd. elements was monitored. It was possible to scan either the entire mass range or a selected no. of isotopes. Reversed-phase chromatog. was used to sep. Zn-contg. species in chicken meat that had been intrinsically and extrinsically labeled with stable isotopes of Zn. The ratio obtained for the intrinsic label agreed with that obtained by other workers using thermal ionization mass spectrometry. Time-resolved anal. permitted rapid data acquisition, thus reducing the no. of chromatog. runs required. However, at present, data handling can be time consuming. Further software developments will add to the advantages that this technique offers.

L10 ANSWER 134 OF 218 CA COPYRIGHT 2000 ACS  
AN 105:107692 CA

TI Direct calibration of GC/MS systems using SRM (Standard Reference Material) gas cylinders

AU Byrd, G. D.; Richie, K. L.; Sniegowski, L. T.; White, E.  
CS Org. Anal. Res. Div., Natl. Bur. Stand. (NML), Gaithersburg, MD, USA  
SO Report (1985), EPA/600/4-85/062; Order No. PB86-110715/GAR, 32 pp. Avail.: NTIS From: Gov. Rep. Announce. Index (U. S.) 1986, 86(4), Abstr. No. 604,988

DT Report *order*  
LA English

AB A cryogenic trapping system was developed for use in calibrating gas chromatog./mass spectrometric (GC/MS) systems for the anal. of volatile org. compds. This system provides for direct Std. Ref. Material (SRM)

traceability on data generated on gaseous samples. The cryogenic trap is a coil of stainless steel tubing immersed in a cryogen to trap and preconcentrate organic species present in a gaseous sample. The trap also contains a heated injection port for the addition of isotopically labeled compounds for use in isotope dilution measurements. The first part of this research is concerned with the development of isotope dilution mass spectrometry as an independent method for the quantification of analytes in gaseous samples to be used as standards. Results are presented for the detection of bromobenzene in nitrogen at nominal concentrations of 1 and 25 ppb. In the second part of the research a calibration curve method was developed for using these standards in auditing the performance of GC/MS systems.

L10 ANSWER 154 OF 218 CA COPYRIGHT 2000 ACS  
AN 99:16090 CA  
TI Isotope cluster chromatography to locate isotopically labeled species  
AU Anderegg, Robert J.  
CS Dep. Chem., Univ. Maine, Orono, ME, 04469, USA  
SO J. Chromatogr. (1983), 275(1), 154-60 CODEN: JOCRAM; ISSN: 0021-9673  
DT Journal  
LA English  
AB The technique of isotope cluster chromatography, which was designed to search gas chromatography-mass spectrometry data sets for mass spectra displaying the isotope cluster patterns resulting from Cl or Br was expanded to include a search for any isotope cluster specified by the user. The products of metabolic or chemical reactions can be quickly located by computer, allowing the investigators to concentrate their time on compounds which have incorporated a stable-isotope label. Although the data presented were all collected as positive ions in the electron ionization mode, the technique would work equally well for chemical ionization and for negative ion mass spectra, provided that the isotope patterns remain undistorted. In addition to drug metabolism studies, the technique can be used in experiments in which a mixture of stable isotope labeled and non-labeled derivatizing reagents is used. In this case, the computer assists in locating the spectra of compounds which contain a particular functional group which has been derivatized by distinguishing such compounds from others which do not display the isotopic doublet.

L10 ANSWER 190 OF 218 CA COPYRIGHT 2000 ACS  
AN 85:186324 CA  
TI Mixture analysis by mass-analyzed ion kinetic energy spectrometry  
AU Kruger, T. L.; Litton, J. F.; Kondrat, R. W.; Cooks, R. G.  
CS Dep. Chem., Purdue Univ., West Lafayette, Indiana, USA  
SO Anal. Chem. (1976), 48(14), 2113-19 CODEN: ANCHAM  
DT Journal  
LA English  
AB The method of mass-analyzed ion kinetic energy spectrometry with both electron impact and chemical ionization was applied to the analysis of mixtures. Separation is achieved by mass analysis and identification by kinetic energy analysis of fragmentation products. Both unimolecular and collision-induced dissociation are employed, the latter being more useful in structure determinations. Sensitivity limits are established as  $\sim 10^{-11}$  g. Quantitative analysis to  $\pm 0.5\%$  is possible with internal standards, and higher accuracy should be possible with isotopically labeled standards. Results are presented for the analysis of mixtures of simple dialkyl ketones, including isomeric compounds; the crude products of a sterically controlled organic reaction; and isotopically enriched species.

L10 ANSWER 199 OF 218 CA COPYRIGHT 2000 ACS  
AN 82:164625 CA  
TI Quantitation of plasma levels of propoxyphene and norpropoxyphene by

combined use of stable isotope labeling and selected ion monitoring  
AU Sullivan, Hugh R.; Emmerson, John L.; Marshall, Frederick J.; Wood, Paul  
G.; McMahon, Robert E.  
CS Lilly Res. Lab., Indianapolis, Indiana, USA  
SO Drug Metab. Dispos. (1974), 2(6), 526-32 CODEN: DMDSAI  
DT Journal *order*  
LA English  
AB A specific and sensitive assay was developed for the detn. of  $\alpha$ -d-propoxy-  
phene (I) [469-62-5] and its principal metabolite, norpropoxyphene  
[32501-12-5], in blood plasma, using deuterium-labeled I and  
norpropoxyphene as internal stds. and gas chromatog.-mass spectrometry.  
Application of the method to propoxyphene-HCl [1639-60-7] metab. in dogs  
and rats indicated that the dog is the more appropriate model for I  
pharmacokinetic studies in man.

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STN INTERNATIONAL LOGOFF AT 13:20:06 ON 16 FEB 2000

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(FILE 'HOME' ENTERED AT 14:49:51 ON 16 FEB 2000)  
FILE 'CA' ENTERED AT 14:49:58 ON 16 FEB 2000  
L1 23317 S INTERNAL STANDARD  
L2 1199 S L1 AND ISOTOP?  
L3 213 S L2 AND(MASS(1A) (ACTION OR BALANCE) OR CALIBRAT? OR CORRECT?)  
L4 178 S L3 AND MASS SPECT?  
L5 35 S L3 NOT L4  
L6 6 S L5 AND(CONTAMINAT? OR MASS FRAGMEN?)  
L7 151 S L4,L6 NOT PY>1997  
FILE 'CAOLD' ENTERED AT 14:59:42 ON 16 FEB 2000  
L8 5 S L2  
L9 10 S L1 AND(MASS(1A) (ACTION OR BALANCE) OR CALIBRAT? OR CORRECT?)

=> d l7 bib,ab 1-151

L7 ANSWER 1 OF 151 CA COPYRIGHT 2000 ACS  
AN 130:10158 CA  
TI Determination of pentachlorophenol (PCP) in samples of the Environmental  
Specimen Bank using isotope dilution  
AU Martens, D.; Prachar, V.; Amberg, S.; Oxynos, K.; Schramm, K.-W.; Kettrup,  
A.  
CS Institute Ecological Chemistry, GSF-National Research Center Environment  
Health, Neuherberg, D-85764, Germany  
SO Int. J. Environ. Anal. Chem. (1997), 68(4), 415-427 CODEN: IJEAA3; ISSN:  
0306-7319  
DT Journal *order*  
LA English  
AB A quick and efficient method for detn. of pentachlorophenol (PCP) in  
various environmental matrixes was developed. The method includes alk.  
hydrolysis of bound PCP, acidification, simultaneous steam distn., and  
extn. in one glass app. After clean-up and derivatization with Ac2O, the  
samples were analyzed by GC/mass spectrometry. Concns. were calcd. using  
13C-labeled PCP as the internal std. Validation was carried out with  
various environmental samples (soil, fish, conifer needles, kale). The  
method can be used for various biol. samples without any modification. The  
exts. are free of matrix components (lipids, chlorophyll, terpenes, etc.)  
and other contaminants, which results in clear chromatograms with few  
peaks. Therefore, correct integration is facilitated. Although the

recoveries of PCP are in the range of 50-90%, due to losses during the several method steps, these losses can be cor. with the  $^{13}\text{C}$ -labeled internal std., resulting in high precision (1.5-2.2% std. deviation).

17 ANSWER 5 OF 151 CA COPYRIGHT 2000 ACS

AN 128:105811 CA

TI Low-temperature pyrolysis of CCA-treated wood waste: chemical determination and statistical analysis of metal input and output; mass balances

AU Helsen, L.; Van Den Bulck, E.; Van Den Broeck, K.; Vandecasteele, C.

CS Department of Mechanical Engineering, Katholieke Universiteit Leuven, Heverlee, 3001, Belg.

SO Waste Manage. (Oxford) (1997), 17(1), 79-86 CODEN: WAMAE2; ISSN: 0956-053X

DT Journal

LA English

AB Low-temp. pyrolysis is proposed as an alternative method to dispose of CCA-treated wood waste. In the frame of a study aiming at optimizing the pyrolysis of CCA-treated wood, an exptl. facility has been built to examine the influence of important process parameters (pyrolysis temp., residence time, heating rate, particle size,) on the release of metals and on the resultant mass redn. In order to perform a mass balance calcn. for the total system, a method for metal anal. was developed. Two leaching procedures and one dissoln. procedure were tested and compared with each other, resulting in an optimal procedure to bring the metals into soln.: "the BSI method" to det. the total amt. of Cr, Cu and As in the dried wood and "the Reflux method" to det. the total amt. of Cr, Cu and As in the pyrolysis residue. These results illustrate that Cr is more strongly bound in the pyrolysis residue as compared to the CCA-treated wood. The anal. technique used was inductively coupled plasma-mass spectrometry, and the anal. problems like interferences and matrix effects were solved by using the appropriate isotope, an internal std., and math. corrections. The resulting optimal technique for CCA-treated wood ("the BSI method") was applied to wood samples with different particle sizes. A statistical anal. of the Cr, Cu, and As content in the CCA-treated wood shows the heterogeneous character of CCA-treated wood samples. Heterogeneity becomes less important when using samples with a small range of particle sizes. The smaller wood particles have significantly higher metal concns. than the larger particles. Realistic mass balances for the metals were obtained and showed that most of the Cr, Cu, and As remained in the pyrolysis residue.

17 ANSWER 12 OF 151 CA COPYRIGHT 2000 ACS

AN 127:75213 CA

TI Different quantification approaches for the analysis of biological and environmental samples using inductively coupled plasma mass spectrometry

AU Alonso, Jose Ignacio Garcia; Camblor, Manuel Gutierrez; Bayon, Maria Montes; Marchante-Gayon, Juan Manuel; Sanz-Medel, Alfredo

CS Department of Physical and Analytical Chemistry, Faculty of Chemistry, University of Oviedo, Oviedo, 33006, Spain

SO J. Mass Spectrom. (1997), 32(5), 556-564 CODEN: JMSPFJ; ISSN: 1076-5174

DT Journal

LA English

AB For the anal. of biol. and environmental materials by inductively coupled plasma mass spectrometry (ICP-MS), several quantification procedures can be used depending on the precision and accuracy required. Semi-quant. methods based on the molar response curve were compared with conventional external calibration and std. addns. for the anal. of waters and sewage sludges. For the anal. of biol. materials, where higher quality data were required, isotope diln. anal. using enriched isotopes was applied. The molar sensitivity for different elements in ICP-MS was a simple function of the

mass of the isotopes measured after normalization for ionization efficiency which could be fitted to a 3rd-order polynomial equation. Element ionization adjustments for the 3rd-order polynomial, using the Saha equation, allowed the calcn. of the plasma ionization temp. and electron d. For the detn. of trace metals in waters and sewage sludges, the samples were spiked with different internal stds., ionization corrections were performed and the results obtained agreed with those obtained by external calibration and std. addns. within a factor of 2 but, on av., the agreement was within 20%. The detn. of Mo in biol. ref. materials was performed by isotope diln. anal. taking into account possible sources of error in the measurements by ICP-MS such as mass discrimination, detector dead time, isobaric interferences and random error propagation.

✓  
AN 126:320793 CA  
TI Reproducibility testing of a sequential extraction scheme for the determination of trace metal speciation in a marine reference sediment by inductively coupled plasma-mass spectrometry  
AU Marin, B.; Valladon, M.; Polve, M.; Monaco, A.  
CS Laboratoire de Sedimentologie et Geochimie Marines, URA 715, Universite de Perpignan, Perpignan, Fr.  
SO Anal. Chim. Acta (1997), 342(2-3), 91-112 CODEN: ACACAM; ISSN: 0003-2670  
DT Journal  
LA English  
AB The sequential extn. scheme procedure recommended by the Bureau Commun de Ref. of the Commission of the European Communities was applied to a ref. marine sediment (Std. Ref. Material, SRM 1646a) to test the reproducibility of the method. Twelve elements (Sc, Cr, Co, Ni, Cu, Zn, Cd, Sn, Ce, Pb, Th, U) in the exts. were detd. by inductively coupled plasma-mass spectrometry. The adopted calibration strategy was external calibration with internal standardization. Measurement of concns. by >1 isotope/element allowed detection and overcame spectral interferences. Internal normalization improved long-term precision, although the internal stds. used appeared not to be the best for the 45-238 mass range of such materials. The sequential extn. procedure was reproducible enough for environmental speciation studies. Sum amts. of trace metals released during the 4 steps were similar to those released by total acid digestion of the sediment.

(L7)  
AN 126:287245 CA  
TI Isotope dilution as a calibration method for solid sampling electrothermal vaporization inductively coupled plasma mass spectrometry  
AU Vanhaecke, Frank; Boonen, Sylvie; Moens, Luc; Dams, Richard  
CS Lab. Analytical Chem., Ghent Univ., Ghent, B-9000, Belg.  
SO J. Anal. At. Spectrom. (1997), 12(2), 125-130 CODEN: JASPE2; ISSN: 0267-9477  
DT Journal *order*  
LA English  
AB The present paper reports on the use of isotope diln. as a method of calibration for solid sampling ETV-ICP-MS. The possibilities and limitations of this calibration strategy were evaluated by detg. the Cd or Se content in solid CRMs of different origin. Since isotope ratios are only slightly affected or not affected at all by (i) matrix effects, (ii) signal drift and instrument instability and (iii) variations in the vaporization and/or transport efficiency, isotope diln. allows accurate analyses to be carried out (mean deviation between solid sampling ETV-ICP-MS results and certified values <10%). The precision attainable is detd. by the sample



homogeneity and is hence comparable to that obtained using other calibration techniques, such as (i) external calibration with either a solid std. or an aq. std. soln. or (ii) std. addns. An important advantage of isotope diln. over the aforementioned calibration techniques for solid sampling ETV-ICP-MS, however, is that the use of an elemental internal std. is no longer required. For some materials, accurate anal. results could not be obtained as at least one of the isotopes involved is subject to spectral interference. The use of several parameters allowing spectral interferences to be detected is discussed. Finally, solid sampling ETV-ICP-MS was used for the detn. of the Cd content in tobacco as a 'real-life' sample and the results obtained using isotope diln. and single std. addn. for calibration were compared with one another and with the result obtained (after taking the ample into soln.) using pneumatic nebulization ICP-MS.

L7 ANSWER 16 OF 151 CA COPYRIGHT 2000 ACS

AN 126:258094 CA

TI Studies of internal standardization in electrothermal-vaporization inductively coupled plasma mass spectrometry (ETV-ICP-MS) with a transversely heated graphite tube

AU Hoffmann, E.; Luedke, C.; Skole, J.

CS Lab. Spektroskopische Methoden Umweltanalytik, Inst. Spektrochemie Angewandte Spektroskopie, Berlin, D-12489, Germany

SO CANAS '95, Colloq. Anal. Atomspektrosk. (1996), Meeting Date 1995, 157-162. Editor(s): Welz, Bernhard. Publisher: Bodenseewerk Perkin-Elmer, Ueberlingen, Germany. CODEN: 64APAD

DT Conference

LA German

AB For the first time, a transversely heated electrothermal vaporizer was used in combination with ICP-MS. A direct and brief connection to the injector tube of the ICP torch provided the condition that only low transport losses of the sample vapor occurred. With this arrangement, one can attain not only an increase in the ion intensity, but one can also decrease the well-known bending of the calibration curves in the lower concn. range, caused by long-term heating of the graphite tubes, with longer lines to the plasma. Moreover, the memory effect is lower. Measurements with Pb and Cd resulted in an improvement in the reproducibility of the anal. signal by internal standardization. In the ETV-ICP-MS, the analyte element itself can also be an internal std., esp. if it possesses >1 stable isotope. The solvents for these analyses were water and HCl solns. *order*

L7 ANSWER 17 OF 151 CA COPYRIGHT 2000 ACS

AN 126:174371 CA

TI A simple method for the precise determination of >40 trace elements in geological samples by ICPMS using enriched isotope internal standardization

AU Eggins, S. M.; Woodhead, J. D.; Kinsley, L. P. J.; Mortimer, G. E.; Sylvester, P.; McCulloch, M. T.; Hergt, J. M.; Handler, M. R.

CS Research School of Earth Sciences, Australian National University, Canberra, Australia

SO Chem. Geol. (1997), 134(4), 311-326 CODEN: CHGEAD; ISSN: 0009-2541

DT Journal

LA English

AB The combination of enriched isotopes and conventional elemental internal stds. permits the precise detn. of >40 trace elements by ICPMS in a broad spectrum of geol. matrixes. Enriched isotopes expand the suite of available ref. isotopes spaced through the mass spectrum, so that the complex mass-dependent variations in sensitivity encountered during ICPMS anal. can be monitored and deconvolved. The method developed is straightforward, entailing simple sample prepn., instrument calibration, *order*

and data redn. procedures, as well as providing extended element coverage, improved precision, and both time and cost benefits compared to alternative anal. strategies. Anal. precision near or better than 1% RSD (relative std. deviation) is achieved for most elements with mass >80 amu and between 1% and 4% (RSD) for elements with mass <80 amu, while maintaining low detection limits (<1 to <10 ng g<sup>-1</sup> for elements with mass >80 amu and <10 ng g<sup>-1</sup> to 1 µg g<sup>-1</sup> for elements with mass <80 amu). The subtle geochem. differences which can be resolved using this method are demonstrated by analyses of Nb, Ta, Zr, and Hf in magmas from ocean islands and subduction zones. These data reveal significant departures from chondritic Zr/Hf and Nb/Ta values, and systematic trends which are consistent with greater incompatibility of Zr relative to Hf and also of Nb relative to Ta during melting of the upper mantle. The occurrence of significantly subchondritic Zr/Hf and Nb/Ta ratios in Nb-poor subduction zone magmas, supports the notion that the depletion of high-field strength elements in subduction magmas is due to their removal from the mantle wedge by prior melting events.

✓  
LV ANSWER 20 OF 151 CA COPYRIGHT 2000 ACS  
AN 126:44528 CA  
TI Calibration for isotope dilution mass spectrometry - description of an  
AU Thienpont, Linda M.; Van Nieuwenhove, Benedikt; Stoeckl, Dietmar; De  
CS Leenheer, Andre P.  
Laboratoria voor Medische Biochemie en voor Klinische Analyse, Universiteit  
Gent, Ghent, B-9000, Belg.  
SO J. Mass Spectrom. (1996), 31(10), 1119-1125 CODEN: JMSPFJ; ISSN: 1076-5174  
DT Journal  
LA English  
AB A calibration method for isotope diln. mass spectrometry is presented that  
fully accounts for non-linearity of calibration functions, caused by the  
interference of the analyte on the m/z used for measurement of the internal  
std. and vice versa. In this way, it is also possible to use incompletely  
labeled mols. of analogs with an mass increment of only 1 u for isotope  
diln., on condition that certain restrictions are respected. In addn., the  
proposed method is less time consuming than bracketing. The method works  
with the computer-stored full calibration curve and a single calibration  
point that is measured daily. The calibration curve is constructed from  
the exptl. detd. mass spectral overlap between the unlabeled analyte and  
the labeled internal std. at the m/z values chosen for measurement.  
Measurement results for samples with unknown analyte concn. are calcd. on  
the basis of a linear relationship between their ion abundance ratio and  
that of the daily single calibration point, but cor. by a factor derived  
from the theor. calibration function. All calcns. are performed with  
commonly available spreadsheet software. An application is presented for  
detg. serum uric acid with a candidate gas chromatog./isotope diln. mass  
spectrometric ref. method.

✓  
LV ANSWER 27 OF 151 CA COPYRIGHT 2000 ACS  
AN 124:115699 CA  
TI Isotope dilution gas chromatographic-mass spectrometric method for the  
AU determination of isoflavonoids, coumestrol, and lignans in food samples  
Mazur, Witold; Fotsis, Theodore; Wahala, Kristina; Ojala, Sirpa; Salakka,  
CS Auli; Adlercreutz, Herman  
Department Clinical Chemistry, University Helsinki, Helsinki, FIN-00290,  
Finland  
SO Anal. Biochem. (1996), 233(2), 169-80 CODEN: ANBCA2; ISSN: 0003-2697  
DT Journal

LA English  
AB The authors present a method for the detn. of the phytoestrogens formononetin, biochanin A, daidzein, genistein, and coumestrol and simultaneously the lignans secoisolariciresinol (SECO) and matairesinol in plant-derived foods. These compds. are measured by isotope diln. gas chromatog.-mass spectrometry in the selected ion monitoring mode (ID/GC/MS/SIM) using synthesized deuterated internal stds. for the correction of losses during the procedure. A three-step hydrolysis - a rehydration with distd. H<sub>2</sub>O, followed by enzymic and acid hydrolysis - was applied in order to convert the diphenolic glycosides into their resp. aglycons. Purifn. and sepn. are carried out in two ion-exchange chromatog. steps followed by derivatization and GC-MS. The within-assay imprecision values vary 3.1-9.6% and the between-assay imprecision 7.0-21.2%. The mean recovery of authentic stds. processed through the whole procedure varied from 95.5 to 105.5%.

✓  
LX ANSWER 31 OF 151 CA COPYRIGHT 2000 ACS

AN 123:238790 CA

TI Measurement of Tl(III/I) Electron Self-Exchange Rates Using Enriched Stable Isotope Labels and Inductively Coupled Plasma Mass Spectrometry

AU Ketterer, Michael E.; Fiorentino, Michael A.

CS Department of Chemistry, John Carroll University, University Heights, OH, 44118, USA

SO Anal. Chem. (1995), 67(21), 4004-9 CODEN: ANCHAM; ISSN: 0003-2700

DT Journal

LA English

AB An approach is described for measuring electron self-exchange rate consts. ( $k_{11}$ ) in soln. based upon stable isotope-labeled reactants, chem. sepn., and inductively coupled plasma mass spectrometry. The technique is demonstrated for the exchange between Tl(III) and Tl(I) aquo ions in aq. HClO<sub>4</sub>. Tl(III) is prepd. using <sup>203</sup>Tl-enriched Tl<sub>2</sub>O<sub>3</sub> (<sup>203</sup>Tl abundance, ~36%), and Tl(I) is prepd. from natural abundance Tl reagents (natural <sup>203</sup>Tl abundance, 29.52%). The exchange is monitored by mixing the labeled and unlabeled reactants and performing timewise sepn. through selective pptn. of Tl(I) as TlBr. Isotope abundances are measured in the TlBr ppt. and Tl(III) soln. phases using ICPMS with minimal sample prepn.; an NIST 981 (common lead) spike is added, and the <sup>208</sup>Pb/<sup>206</sup>Pb is measured as an internal std. to correct for mass discrimination. The self-exchange rate const. is detd. from a McKay plot obtained from the <sup>205</sup>Tl abundances of either oxidn. state. A  $k_{11}$  of  $(1.0 \pm 0.1) \times 10^{-4} \text{ M}^{-1} \text{ s}^{-1}$  was obtained in 1.5 M aq. HClO<sub>4</sub> at 25 °C. The obtained  $k_{11}$  compares favorably to a value of  $1.1 \times 10^{-4} \text{ M}^{-1} \text{ s}^{-1}$  based upon a previously published study of this exchange reaction using radiolabeled (<sup>204</sup>Tl) reactants.

✓  
LX ANSWER 34 OF 151 CA COPYRIGHT 2000 ACS

AN 123:24842 CA

TI Determination of Elemental Content of Rocks by Laser Ablation Inductively Coupled Plasma Mass Spectrometry

AU Lichte, Frederick E.

CS Denver Federal Center, U.S. Geological Survey, Denver, CO, 80225, USA

SO Anal. Chem. (1995), 67(14), 2479-85 CODEN: ANCHAM; ISSN: 0003-2700

DT Journal

LA English

AB A new method of anal. for rocks and soils is presented using laser ablation inductively coupled plasma mass spectrometry. It is based on a lithium borate fusion and the free-running mode of a Nd/YAG laser. An Ar/N<sub>2</sub> sample gas improves sensitivity 7× for most elements. Sixty-three elements are characterized for the fusion, and 49 elements can be quantified. Internal

stds. and isotopic spikes ensure accurate results. Limits of detection are 0.01  $\mu\text{g/g}$  for many trace elements. Accuracy approaches 5% for all elements. A new quality assurance procedure is presented that uses fundamental parameters to test relative response factors for the calibration.

✓  
K7 ANSWER 40 OF 151 CA COPYRIGHT 2000 ACS

AN 122:127867 CA

TI Precise determination of isotopic ratios for some biologically significant elements by inductively coupled plasma mass spectroscopy

AU Koirtyohann, S. R.

CS Dep. Chem., Univ. Missouri, Columbia, MO, 65211, USA

SO Spectrochim. Acta, Part B (1994), 49B(12-14), 1305-11 CODEN: SAASBH;  
ISSN: 0584-8547

DT Journal

LA English

AB Isotope ratios for copper, iron, lead, lithium, nickel and zinc were measured with an ELAN 5000 ICP-MS instrument. Except for lithium isotopes, ratio relative std. deviations (RSDs) of about 0.1% were achieved with measurement times of 10 min or less per sample on isotope pairs that differed by no more than a factor of 10 in abundance. It was necessary to accumulate several million counts to reduce statistical counting errors, to correct for the dead time in the counting circuitry, and to compensate for a slow drift of apparent ratios with time. Drift compensation was achieved by using a third isotope of the test element, by adding two internal std. elements with isotopes bracketing the mass range of interest, or by frequent recalibration with a std. of known abundances. Attempts to compensate for drift in lithium isotope ratios were not successful and typical RSDs for  $6\text{Li}/7\text{Li}$  remained around 0.5%. Copper and zinc ratios were measured in pig feces with ratio precision and drift behavior essentially identical to that seen for synthetic solns.

QD95.A1

L7 ANSWER 42 OF 151 CA COPYRIGHT 2000 ACS

AN 122:121939 CA

TI Conceptions and misconceptions in stable isotope dilution. Fundamental mathematical considerations

AU Sabot, J. F.

CS Lab. Chimie Analytique II, Inst. Sciences Pharmaceutiques Biologiques, Lyon, 69373, Fr.

SO Analisis (1994), 22(8), 381-91 CODEN: ANLSCY; ISSN: 0365-4877

DT Journal

LA French

AB The combination of gas chromatog. and mass spectrometry enables the detection and the quant. anal. of various compds. Isotope diln. mass spectrometry proved to be an accurate and precise technique meeting the requirements of abs. or ref. methods. Selected ion monitoring is used to monitor the gas effluents. The calibration graph indicates the ratio of peak-intensities to defined masses against the ratio of the quantities of labeled and unlabeled compds. When a labeled mol. is used as an internal std. in a ref. method, or as a tracer in pharmacol. or in biochem., two different cases of isotope diln. are encountered. Corresponding characteristic equations are dissected and explained. The graphs have a hyperbolic form in which the lower parts can be linearized. This paper describes the math. approach of present data acquisition and assesses the extent to which accuracy can be obtained in practice. Calcn. procedures are described and the limits of linearization are defined.

✓  
K7 ANSWER 45 OF 151 CA COPYRIGHT 2000 ACS

AN 121:101332 CA  
 TI Determination of lead by flow-injection inductively coupled plasma mass spectrometry comparing several calibration techniques  
 AU Goossens, Jan; Moens, Luc; Dams, Richard  
 CS Laboratory of Analytical Chemistry, Institute for Nuclear Sciences, Ghent University, Proeftuinstraat 86, Ghent, B-9000, Belg.  
 SO Anal. Chim. Acta (1994), 293(1-2), 171-81 CODEN: ACACAM; ISSN: 0003-2670  
 DT Journal  
 LA English  
 AB In this paper the authors have evaluated the coupling of a modular flow-injection system to an inductively coupled plasma mass spectrometer for lead detns. by direct anal. of wines and urine samples. The flow-injection system used allows an online sample diln. and an online addn. of internal std. and calibrant soln. It was found that particular attention should be paid to the adjustment of the nebulizer gas flow rate in order to obtain max. sensitivity and precision. In this way and for the exptl. set-up described, R.S.D. values  $\leq 1\%$  on the  $^{208}\text{Pb}^+$  signal for 5 consecutive injections could readily be achieved. The relative merits of external calibration, std. addns. and isotope diln. for the calibration of the transient lead signals were compared. It appeared that from the viewpoint of accuracy, precision and flexibility, the std. addns. method is the most preferable procedure. Further, it was found that the precision of isotope ratio detns. is degraded in comparison to continuous nebulization. However, matrix-induced mass fractionation on the lead isotope ratios as obsd. for the continuous nebulization of an aq. ethanolic (wine) matrix did not occur in flow-injection anal. The quantitation of lead by direct anal. of undiluted wine and urine samples using this flow-injection method in combination with std. addns. calibration resulted in very accurate results (compared to certified and ref. values). Excellent relative std. deviations (for 5 consecutive detns.) were obtained ranging from 1% (50  $\mu\text{g/L}$  Pb in white wine) to 5% (3.6  $\mu\text{g/L}$  Pb in urine).

L7 ANSWER 54 OF 151 CA COPYRIGHT 2000 ACS  
 AN 119:39874 CA  
 TI Quantitative trace analysis by combined chromatography and mass spectrometry using external and internal standards  
 AU Boyd, R. K.  
 CS Inst. Mar. Biosci., Natl. Res. Counc., Halifax, NS, B3H 3Z1, Can.  
 SO Rapid Commun. Mass Spectrom. (1993), 7(4), 257-71 CODEN: RCMSEF; ISSN: 0951-4198  
 DT Journal; General Review *under*  
 LA English  
 AB A review with 31 refs. This review covers established methods for trace org. anal. by quant. chromatog. Although these methods are of more general applicability, they are widely used in practice with mass spectrometric detection. In the important class of methods employing surrogate internal stds. (usually isotopically labeled versions of the target analytes), mass spectrometry is almost always obligatory in view of the inability to chromatog. resolve such a std. from the analyte in all but a few exceptional cases. The relative strengths and weaknesses of the methods are compared, and distinctions are drawn between "best" methods for different circumstances, e.g., quality control of pharmaceutical preps. compared with analyses of environmental samples.

*✓* L7 ANSWER 55 OF 151 CA COPYRIGHT 2000 ACS  
 AN 119:33989 CA  
 TI The use of an enriched isotope as an on-line internal standard in inductively coupled plasma mass spectrometry: a reference method for a

proposed determination of tellurium in industrial waste water by means of graphite furnace atomic absorption spectrometry

AU Klinkenberg, Huub; Beeren, Ton; Van Borm, Werner; van der Linden, Fons; Raets, Mich

CS Dep. PAC, DSM Res., Geleen, 6160, Neth.

SO Spectrochim. Acta, Part B (1993), 48B(5), 649-61 CODEN: SAASBH; ISSN: 0584-8547

DT Journal

LA English

AB The continuous addn. of a soln. of an enriched  $^{125}\text{Te}$  as internal std. is used in an online isotope diln. inductively coupled plasma mass spectrometry (ID-ICP-MS) anal. for the detn. of Te in industrial wastewater. The method has the precision and accuracy attainable with isotope diln. In order to check for possible polyat. interferences, 2 analyte isotopes ( $^{128}\text{Te}$  and  $^{130}\text{Te}$ ) were used. Isotopic ratios were converted into calibration graphs that are curved for both analyte isotopes. A formula is presented, with which the shape of a calibration graph can be calcd. beforehand. ICP-MS has been used as a ref. method for a proposed graphite furnace at. absorption spectrometry (GFAAS) procedure that uses the combination of Pd, Triton X-100 and H as matrix modifier. Only Triton X-100 could assure the uniform atomization of Te. Obviously, the particle size distribution of Pd is much more important than the dispersion of Pd particles in the graphite furnace. Forty-eight wastewater samples were analyzed. The GFAAS and ICP-MS results were compared as paired samples using a t-test on their differences. At a confidence level of 0.05, both methods gave identical results.

✓  
IV ANSWER 57 OF 151 CA COPYRIGHT 2000 ACS

AN 118:224797 CA

TI Determination of platinum in urine, ultrafiltrate, and whole plasma by isotope dilution gas chromatography-mass spectrometry compared to electrothermal atomic absorption spectrometry

AU Aggarwal, Suresh K.; Gemma, Nicholas W.; Kinter, Michael; Nicholson, James; Shipe, James R., Jr.; Herold, David A.

CS Health Sci. Cent., Univ. Virginia, Charlottesville, VA, 22908, USA

SO Anal. Biochem. (1993), 210(1), 113-18 CODEN: ANBCA2; ISSN: 0003-2697

DT Journal

LA English

AB Isotope diln. gas chromatog.-mass spectrometry (GC-MS) and electrothermal at. absorption spectrometry (EAAS) are compared for platinum (Pt) detn. in urine, plasma ultrafiltrate, and plasma samples from a patient undergoing cisplatin therapy. The isotope diln. GC-MS method is based on the use of lithium bis(trifluoroethyl)dithiocarbamate as a chelating agent and enriched  $^{192}\text{Pt}$  as an internal std. Pt isotope ratios were measured using a Finnigan MAT 8230 org. mass spectrometer, and Pt concns. were calcd. from different sets of isotope ratios in the mol. ion of the Pt-chelate. In the EAAS method, Pt concns. were detd. using three different approaches. These were (i) calibration curve based on aq. stds. contg. Pt in 10% HCl, (ii) std. addn., and (iii) matrix digestion followed by std. addn. Good agreement was obtained for Pt concns. detd. by GC-MS and EAAS in urine samples while there were significant differences in Pt concns. of ultrafiltrate and whole plasma samples by the two methods. Discussion of possible reasons for these differences emphasizes the need for future crit. evaluation of these methods.

✓  
IV ANSWER 58 OF 151 CA COPYRIGHT 2000 ACS

AN 118:204463 CA

TI Comments on "Isotope dilution liquid chromatography/mass spectrometry using

a particle beam interface"

AU Stoeckl, Dietmar  
CS INSTAND e.V., Duesseldorf, W-4000/1, Germany  
SO Anal. Chem. (1993), 65(10), 1489 CODEN: ANCHAM; ISSN: 0003-2700  
DT Journal  
LA English

AB A polemic in response to D. Doerge et al. (ibid. 1992, 64, 1212). The accuracy of an isotope diln. quantification depends not only on the correct calibration and calcn. procedure, but in the first instance on the accuracy of the exptl. obsd. isotope ratios, which itself depends on instrument features and on the actual values obsd. Best accuracy is obtained with analyte/internal std. (IS) ratios of 1. When the ratio tends to zero or infinity, the reliability of the measurement decreases. Further, the accuracy of isotope diln. measurements decreases with the increase of spectral overlap between analyte and IS. This is shown on analyte/IS mixts., with the following relative intensities on M+/M+1+: analyte 100%/21%, IS 100%/60%, 60%/100%, and 0%/100%.

L7 ANSWER 62 OF 151 CA COPYRIGHT 2000 ACS  
AN 118:138967 CA

TI Mass transport and calibration in liquid chromatography particle beam mass spectrometry

AU Ho, James S.; Behymer, Thomas D.; Budde, William L.; Bellar, Thomas A.  
CS Environ. Monitor. Syst. Lab., U.S. Environ. Protect. Agency, Cincinnati, OH, USA

SO J. Am. Soc. Mass Spectrom. (1992), 3(6), 662-71 CODEN: JAMSEF; ISSN: 1044-0305

DT Journal  
LA English

AB Differences in the designs of two liq. chromatog. particle beam mass spectrometry systems result in differences in the transport of ammonium acetate and differences in ion abundance-enhancing carrier effects. The effect of mobile phase compn., esp. the proportion of water in the mobile phase, on transport efficiency is described. Instrument detection limits for 12 compds. with two different interface designs are presented. The calibrations are generally nonlinear explained in terms of mass transport effects and supported by expts. with isotopically labeled species that coelute with the native species. Summary results of a small multilab. study are presented. Calibration with isotopically labeled internal stds. is recommended for real-world environmental samples.

L7 ANSWER 74 OF 151 CA COPYRIGHT 2000 ACS  
AN 116:227360 CA

TI Isotope dilution liquid chromatography/mass spectrometry using a particle beam interface

AU Doerge, Daniel R.; Burger, Mike W.; Bajic, Steve  
CS Dep. Environ. Biochem., Univ. Hawaii, Manoa, HI, 96822, USA  
SO Anal. Chem. (1992), 64(11), 1212-16 CODEN: ANCHAM; ISSN: 0003-2700  
DT Journal  
LA English

AB The use of a particle beam (PB) interface for quantitation by isotope diln. LC/MS was investigated. Coelution of single-labeled internal stds. (IS) with native compds. caused enhancement of the IS signal. The magnitude of enhancement for [3-13C]caffeine was affected by several exptl. parameters, but no differences were obsd. in the 12C/13C response ratios under these conditions or upon analyte introduction via a gas chromatog. (GC) interface. No elution enhancement was obsd. with [1,3,7-13C3]caffeine, demonstrating that mass transfer effects and chem. complex formation do not

affect PB transmission efficiency. Spectral overlap between native analyte and IS peaks and nonlinear detector response cause the obsd. coelution enhancement. These results confirm that PB/LC/MS does not have inherent limitations for use in isotope diln. expts. as they have been performed by GC/MS. An equation was derived that permits accurate calcn. of isotope diln. results using a single- or multiple-labeled IS. Application of this equation could allow expansion of the isotope diln. technique performed by PB/LC/MS or GC/MS to include single-labeled IS compds. without the ned for nonlinear regression anal. of calibration curves. The method was used for detg. caffeine in coffee products.

IV ANSWER 77 OF 151 CA COPYRIGHT 2000 ACS

AN 116:187285 CA

TI Relative response ratios for dual-isotope measurements via coelution and GC/MS

AU Thomas, Lawrence C.; Weichmann, Walter

CS Dep. Chem., Seattle Univ., Seattle, WA, 98122, USA

SO Talanta (1992), 39(3), 201-6 CODEN: TLNTA2; ISSN: 0039-9140

DT Journal

LA English

AB Dual-isotope internal std. measurements by GC/MS which mimic isotope diln. may suffer from nonlinear response relations, irreproducibilities or unduly large uncertainties because of variations in ionization efficiencies for the resp. isotopic forms in the MS source. Such variations may sometimes be avoided via extensive pretreatments, high resoln. GC sepns. and careful control of instrumental parameters. However, an alternative approach is feasible which instead exploits advantages of decreasing GC resoln. By forcing both forms of each analyte to coelute, their relative ionization efficiencies in the MS source should be nearly const., thereby effectively allowing for const. relative sensitivities over several orders of magnitude in concn. Thus, const. relative response ratios, required for internal std. calcns., may be attained as a consequence of dramatically lowered GC resoln. Coelution results described herein show linear relative sensitivity relations over much broader ranges than obsd. for corresponding conventional calibrations with sepd. components. Coelution methods for dual-isotope GC/MS detns. are compatible with internal std. calcns. and thereby offer a powerful alternative to the conventional approach of requiring expensive and labor-intensive addnl. pretreatments and sepns. to assure resoln. of measured eluates.

L ANSWER 84 OF 151 CA COPYRIGHT 2000 ACS

AN 115:84484 CA

TI Determination of germanium, palladium and platinum in highly concentrated solutions of phosphoric acid and ammonium nitrate by flow injection inductively coupled plasma mass spectrometry (FI-ICP-MS)

AU Peng, Zicheng; Klinkenberg, H.; Beeren, T.; Van Borm, W.

CS Dep. Phys. Anal. Chem., DSM Res., Geleen, 6160 MD, Neth.

SO Spectrochim. Acta, Part B (1991), 46B(6-7), 1051-61 CODEN: SAASBH; ISSN: 0584-8547

DT Journal

LA English

AB Trace germanium, palladium and platinum in a soln. contg. 1.5M (25% mass/vol.) phosphoric acid and 1.5 M (12% mass/vol.) ammonium nitrate have been detd. by flow injection-inductively coupled plasma-mass spectrometry (FI-ICP-MS) using an internal std. and a std. addn. method. By choosing a suitable sampler and skimmer set to eliminate interferences each element could be detd. by two different isotopes:  $^{72}\text{Ge}$ ,  $^{105}\text{Pd}$ ,  $^{108}\text{Pd}$ ,  $^{194}\text{Pt}$  and  $^{195}\text{Pt}$ . The detection limits of the isotopes are 1, 0.2, 0.3, 0.2, 0.3 and



0.3 ng/mL, resp. The relative std. deviation for all isotopes is less than 10% for concns. above 20 ng/mL. The method provided an efficient matrix correction and stable operating conditions for ICP-MS.

17 ANSWER 86 OF 151 CA COPYRIGHT 2000 ACS

AN 114:246308 CA

TI External-source contamination during extraction-distillation in isotope-ratio analysis of soil inorganic nitrogen

AU Chen, Deli; Chalk, Phillip M.; Freney, John R.

CS Sch. Agric. For., Univ. Melbourne, Parkville, 3052, Australia

SO Anal. Chim. Acta (1991), 245(1), 49-55 CODEN: ACACAM; ISSN: 0003-2670

DT Journal

LA English

AB The sources of contamination introduced during the extn., distn., and drying phases of isotope-ratio anal. of soil inorg. nitrogen (ammonium and nitrite + nitrate) were identified, and the individual amts. of contaminants were quantified by isotope diln. The procedure involves addn. of internal std. solns. of  $^{15}\text{N}$ -labeled ammonium and nitrite to reagent blanks which are carried through each stage of the anal. at the same time as the test samples. Potassium chloride extractants, filter-papers, distn. reagents, and atm. ammonia all contributed to diln. of the sample  $^{15}\text{N}$ . Some materials tested contained sufficient contaminants to cause large errors in the detn. of sample  $^{15}\text{N}$  abundance. Both the amt. and isotopic compn. of contaminants can be detd. by the isotope-diln. procedure, which permits the measured sample  $^{15}\text{N}$  abundance to be cor. for contamination.

18 ANSWER 149 OF 151 CA COPYRIGHT 2000 ACS

AN 78:92030 CA

TI Precision of quantitative analysis methods in spark mass spectrometry

AU Ordzhonikidze, K. G.; Samadashvili, O. A.; Glinskikh, V. M.; Yur'eva, O. K.; Karpenko, I. K.

CS USSR

SO Zh. Anal. Khim. (1972), 27(12), 2310-13 CODEN: ZAKHA8

DT Journal

LA Russian

AB The accuracy of spark mass spectrometry results depend to a large degree on the method of calibrating the photoemulsion. The method proposed by J. Kai and M. Miki (1964) is rapid but is not very precise. The calcn. method of R. Stefani et al. (1965), based on the calibration of the photoemulsion by the 2 lines method, gives accurate results, but an internal std. with a known isotope compn. is needed. C. Hull's method (1966) gives the highest precision and is used for mech. evaluation of results. The methods were compared based on the anal. of a Mo matrix for Cr and Fe admixts. from the point of reproducibility of results, rapidity, and simplicity of the mass spectrogram manual treatment. The precision varies from 5-50% with the respect to the std. deflection depending on the method used.

=> d 18 all 1-5

18 ANSWER 4 OF 5 COPYRIGHT 2000 ACS

AN CA57:362a CAOLD

TI Internal-standard technique for precise isotopic abundance measurements in thermalionization mass spectrometry

AU Dietz, Leonard A.; Pachucki, C. F.; Land, G. A.

=> d 19 all 1-10

*Anal chem, 1962, 34, 709-710*

L9 ANSWER 4 OF 10 COPYRIGHT 2000 ACS

AN CA58:10710d CAOLD  
TI Evaluation of calibration data-variable internal standard method  
AU Calder, Allan B. *spectrochim Acta 1959 280-283*  
L9 ANSWER 5 OF 10 COPYRIGHT 2000 ACS  
AN CA57:4967g CAOLD  
TI Reassessment of calibration and computation methods-variable internal  
standard technique  
AU Calder, Allan B.  
L9 ANSWER 7 OF 10 COPYRIGHT 2000 ACS  
AN CA55:20756h CAOLD  
TI Variable internal standard calibration  
AU Chamberlain, G. T.

=> log y

STN INTERNATIONAL LOGOFF AT 15:01:32 ON 16 FEB 2000

=> d his

(FILE 'HOME' ENTERED AT 12:22:57 ON 17 FEB 2000)

FILE 'CA' ENTERED AT 12:23:08 ON 17 FEB 2000

L1 35986 S (SELF OR ELECTRON) (1A) EXCHANG? OR REDOX (1A) COUPL?  
L2 612 S L1 AND ISOTOP?  
L3 41 S MASS SPEC? AND L2 NOT PY>1997

=> d bib, ab 1-41

L4 ANSWER 1 OF 41 CA COPYRIGHT 2000 ACS  
AN 126:109432 CA  
TI Determination of Aqueous FeIII/II Electron Self-Exchange Rates Using  
Enriched Stable Isotope Labels, Ion Chromatography, and Inductively Coupled  
Plasma Mass Spectrometry  
AU Kozerski, Gary E.; Fiorentino, Michael A.; Ketterer, Michael E.  
CS Department of Chemistry, John Carroll University, University Heights, OH,  
44118, USA  
SO Anal. Chem. (1997), 69(4), 783-788 CODEN: ANCHAM; ISSN: 0003-2700  
LA English  
AB A strategy is described for rapid online measurement of electron self-  
exchange rates between aq. FeIII and FeII in aq. soln. using stable <sup>57</sup>Fe-  
labeled reactants, cation chromatog., and inductively coupled plasma mass  
spectrometry. The self-exchange is monitored by mixing the reactants and  
performing time-wise sepns. of FeII and FeIII ions. Sepns. are completed  
in 30-60 s using a weak phosphonic/carboxylic acid cation exchange guard  
column and 0.1-0.5 M aq. HClO<sub>4</sub> eluent. The resulting time series of <sup>56</sup>Fe  
and <sup>57</sup>Fe chromatograms display systematic changes in isotopic abundances  
from which the self-exchange rate const., k<sub>11</sub>, is obtained. Two different  
schemes are used for mixing and sampling the reaction mixt.; using a  
peristaltically pumped flow reactor, reaction half-lives on the order of 30  
s can be monitored. A series of k<sub>11</sub> results are obtained under a variety  
of temp. (2.0, 21.6, and 25.0 .degree.C) and ionic strength conditions  
(0.10, 0.50, and 0.55 M aq. HClO<sub>4</sub>) which are congruent with three  
previously published radiolabeling studies for this reaction.

=> log y

STN INTERNATIONAL LOGOFF AT 12:25:50 ON 17 FEB 2000